

The X6A Scientific Advisory Committee (SAC) to the NSLS, met on February 19th to evaluate the progress made by the NIGMS Facility during the calendar year 2006. The X6A facility is solely funded by the NIGMS and the committee was charged to assess the facility's scientific and technical progress. The report below reflects the opinions of the members of the SAC, Dr. Mario Amzel (chair), John Hopkins University, Dr. Leemor Joshua-Tor, Cold Spring Harbor, and Dr. Craig Ogata (Advanced Photon Source).

Over the past year the X6A beam line became more established. The actual expansion is outstanding, with over 100% of user scheduled beam time the beam line has to be considered oversubscribed. Clearly the X6A team managed to succeed where other bending magnet beamlines failed: increasing their user base at a time in which users try to carry out all their experiments on ID beamlines. Two groups, Dr. Ya Ha, Yale University and Dr. G. Snell, Takeda San Diego, represented the X6A user base, commending the X6A staff for being goal oriented, interested in continuous improvements and providers of excellent user support. Users that prefer this beamline come because of the extensive support they get. Indeed most of the X6A users are naive users, from non-expert labs, which are very unfamiliar with crystallographic techniques. The support and atmosphere at X6A is very amenable for this growing type of user.

It appears that the investment that was made by the NIGMS really paid off given the marked increase in productivity shown by the X6A beamline. The number of publications and PDB depositions, from this beamline was higher over the last year than that observed for other NSLS bending magnet beam lines. With the largest number of publications (36, 19 in journals with an impact factor > 6.0) amongst bending magnet beam lines X6A is not very far behind the NSLS ID lines with 59 and 48 publications. This is a remarkable increase at a time when most if not all other bending magnet beamlines are showing a marked decline in productivity. The beam line also has very significant high-end publications including, for example, the romboïd structure published by Ha and colleagues in Nature. This was the first of 4 other publications on the same structure and the easy access and support from the beamline staff greatly facilitated this. They also have some very productive industrial users that do not publish or deposit their structures in the PDB, but the committee was very impressed with the number of useful data sets collected at X6A. We heard a report from one industrial user that noted that their productivity on X6A is on par with their productivity on their dedicated beamline at ALS. Of utmost importance to

the X6A user is the arrangement between X6A and the X29 ID beamline. Investigators that have beam time in X6A can move to X29 for a short shift to complete data collection. This is a very important and productive synergetic arrangement.

One problem that was noted by the staff is that not all users report their use of X6A in their publications or PDB depositions. This is because they often use X6A for initial data collection and screening and then collect their final data on an insertion device beamline. In the publication Users usually report only on the beamline where the final data set(s) were collected. In addition PDB does not provide enough space to report on all the beamlines that were used for the study. However, we note that work on the bending magnet lines to sort out problems is crucial for many projects.

The small X6A staff has cleverly taken advantage of the technical expertise of the NSLS staff, as well as drawn in technical and scientific support from other facilities. Through the groups lead by D. P. Siddons and S. Hulbert the team at X6A has greatly enhanced their capabilities by leveraging their capabilities in terms of implementing technologies, such as detectors etc., well beyond the support provided by the NIGMS. The X6A group led by V. Stojanoff decided to take advantage of the expertise and experience of T. Earnest's group at the ALS by procuring their sample automounter. In addition to the purchase of the hardware, they have adopted the Blu-Ice like GUI/DCS system developed at the ALS. This allowed the group to quickly adapt their EPICS/VME, Compumotor, Galil and Wago control system into a unified system. The focus of the group was clearly on the use of the system. Due to these early decisions, and the careful selection of a very experienced user (G. Snell) their automated sample changer has moved quickly past the commissioning stage. Snell has been the primary user of the robot in the early stages of operation. In his three trips to the X6A facility he has documented the progress of the development of the robot. The close working relationship of the staff and the expert-user has resulted in 790 crystals screened and 90 data sets collected, averaging 22 crystals tested and 2.3 data sets collected per shift with a structure success rate of 33%, comparable with the throughput performance observed by the group at other facilities. Snell presented this data in a strong endorsement to the operation of the Automounter at X6A. The group lists their reason for using this beamline as: implementation of the ALS-Automounter, smooth operation, and excellent centering algorithm. As result of the synergistic relation between the group of Dr. Snell and the X6A staff several improvements to the beam line were

suggested:

1. Airbearing Goniometer stage. The rate limiting step in autocentering is the rotation around the spindle axis. Replacing the stepping motor axis by an airbearing goniometer stage will reduce significantly the autocentering time.
2. Improve crystal viewing optics. In-line viewing, multiple views, and variable magnification.

This committee notes two important developments at X6A that are unique to this beamline and could be exported elsewhere:

1. The crystal autocentering software, CrysCent. Two other autocentering utilities are currently available, but these do not even approach the very high success rate that CrysCent achieves. For a very small investment, namely a summer student (applied physics major), this resource was able to develop and implement this very useful software. This also allows NSLS to better interact with other facilities to exchange ideas and utilities. The group has recently submitted a paper on this development. This also exemplifies the strength of this group and their wisdom in implementing software and hardware from other sources when available but using their expertise to develop something completely new to enhance their performance.
2. The group continued demonstrating ingenuity and creativity in the development of their internet services. Over the past year they adopted Media Wiki as the primary environment for their website. Unique are the user beamtime SELF-scheduling tools, reporting and administrative tools, and real time tracking tools. It was developed and implemented extremely efficiently by Kun Qian, one of the X6A staff members. This is a wonderful and unique tool and other facilities should take note! It is hard to overstate the ease, effectiveness and the amount of time and aggravation saved both from the user and the staff by using the self-scheduling feature.

There are four staff members at X6A. They are all very effective in the unique aspects of X6A. Staff members are encouraged by the NSLS management to pursue their own research projects. The X6A staff is no exception, as exemplified by the excellent presentations by J. Jakoncic on the structure and mechanism of a dioxygenase involved in the metabolism

of poly aromatic hydrocarbons, and M. Allaire on the studies of TonB in complex with FhuA the transporter of ferrichrome. Research by beam line personnel assures the high standard of user support at this Facility and should be encouraged and fostered. Furthermore it permits the NSLS to retain outstanding personnel with clear scientific vision by establishing a career path for the staff.

One of the unique aspects of this facility is the one-on-one assistance received by the inexperienced user. Developed as part of the group's strategy to attract users to the X6A beamline "The X6A Workbench: Advanced Tools in Structural Biology" is a hands-on course that was developed specifically for those members of the community who are not familiar with the synchrotron methods in structural biology. This is a useful service to the structural biology community that should be continued and supported.

The committee is concerned that the year-by-year type of support from NIGMS, rather than a multi-year grant, makes it hard to have any kind of long-term vision or enable long-term developments for this beamline.